Supplementary information

Properties and growth of large single crystal of one dimensional organic lead iodine perovskites

Yiming Wang[a], Yanliang Liu[a], Yizhang Wu[a], Junjie Jiang[a], Chunlin Liu[b], Wenlong Liu[b], Kaige Gao[b*], Honglin Cai[a], Xiaoshan Wu[a*]

a. Collaborative Innovation Center of Advanced Microstructures, Laboratory of Solid State Microstructures, School of Physics, Nanjing University, Nanjing 210093, P. R. China.

b. College of Physical Science and Technology, Yangzhou University, Jiangsu 225009, P. R. China

Experimental

Synthesis

0.5 mmol Benzylamine and 1 mmol PbI_2 were mixed in 10ml DMF. Then 5ml hydroiodic acid (57% wt) was dropped to the solution. 2 ml 50% phosphorous acid solution was added to stabilize hydroiodic acid. A clear yellow solution was formed finally. Large single crystals of $DMAPbI_3$ were acquired by evaporation of the solution at room temperature for about two weeks.

Measurement Section.

The elemental analysis was recorded on a Heraeus CHN-0-Rapid elemental analyser. The absorption spectrum was measured by a PV Measurements Model QEX10 through using Integral Sphere Method from 300nm to 1100nm. The single crystal X-ray diffraction was measured by a Bruker D8 QUEST. Powder X-ray diffraction (PXRD) was measured on a Rigaku D/MAX 2000 PC X-ray diffractometer. DSC measurements of single crystals were recorded by using a NETZSCH DSC 200F3 in the temperature range of 100–300 K. The complex permittivity was measured using a Tonghui TH2828A LCR meter. The photoluminescence spectra were detected by time resolved fluorescence spectra (FLSP20, Edinburgh, lhstrcamenss). The absorption spectra were measured by Quantum efficiency tester. Raman spectra were collected using a Horiba Jobin Yvon HR800 spectrometer device by means of a 488 nm laser line. P−E hysteresis loops were recorded on a Precision Premier II (Radiant Technologies, Inc.) using Sawyer-Tower Circuit.

Elemental analysis: To ascertain the structure and purity of compounds $DMAPbI_3$,we quantitatively measured the mass fractions of carbon, and nitrogen in the compound by means of CHN elemental analysis. The results are C 3.91%, N 2.11% for the compound , which are coincident with the theoretical values (C 3.79, N 2.21%). The measurement error of the mass fractions is about 0.3%.

Table S1. Xprep information of the $DMAPbI_3$ single crystal XRD data measured at room temperature.

Option	Space Group	No.	Type	Axes	CSD	R(sym)	N(eq)	Syst. Abs.	CFOM
[A]	P-31c	#163	centro	1	23	0.075	1490	0.8 / 5.6	10.32
[B]	P31c	#159	non-cen	1	12	0.075	1490	0.8 / 5.6	14.73
[C]	P6(3)mc	#186	non-cen	1	21	0.080	1665	0.8 / 5.6	12.77
[D]	P6(3)/mmc	#194	centro	1	16	0.080	1665	0.8 / 5.6	13.22
[E]	P-62c	#190	non-cen	1	11	0.080	1665	0.8 / 5.6	16.56

Table S2 Crystallographic data

Temperature	100 K	293 K
Formula	$C_2NH_8PbI_3$	$C_2NH_8PbI_3$
Formula weight	633.98	633.98
Crystal system	monoclinic	hexagonal
Space group	$P2_1$	$P6_3/mmc$
a / Å	8.9303(6)	8.7799(12)
b / Å	14.6910(9)	8.7799(12)
c / Å	7.9790(5)	8.193(2)
α / °	90	90
β / °	95.994(4)	90
γ / °	90	120
V / Å^3	1041.08(11)	546.94(19)
Z	4	2
D_c / g·cm^{-3}	4.045	3.850
F(000)	1072	520
GOF on F^2	1.035	1.200
$R1$,$wR2$ [$I > 2\sigma(I)$]	0.0716, 0.1781	0.0413, 0.0946
$R1$,$wR2$ (all data)	0.0966, 0.1925	0.0573, 0.1002
Flack parameter	0.470(18)	None

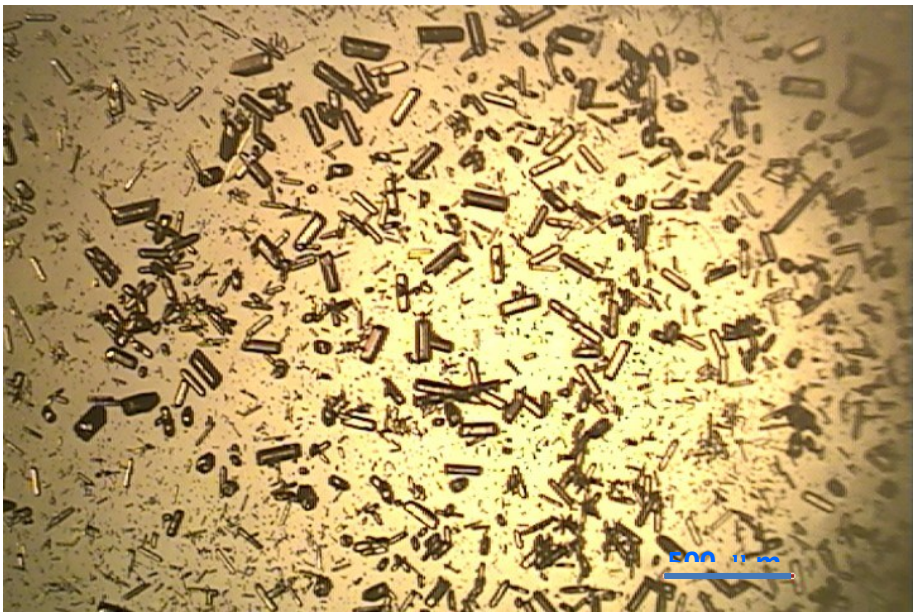

Fig. S1 Microscope photo of 1D $DMAPbI_3$ single crystals with regular shape at the beginning of the growth.

Fig. S2 Microscope photo of 1D $DMAPbI_3$ single crystals with irregular shape.

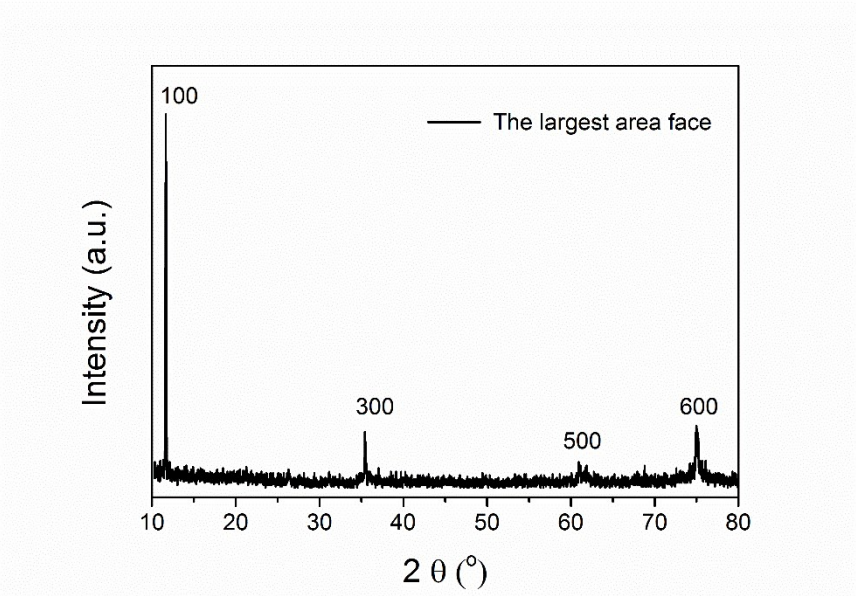

Fig. S3 XRD of the largest area face of single crystal $DMAPbI_3$ at room temperature.

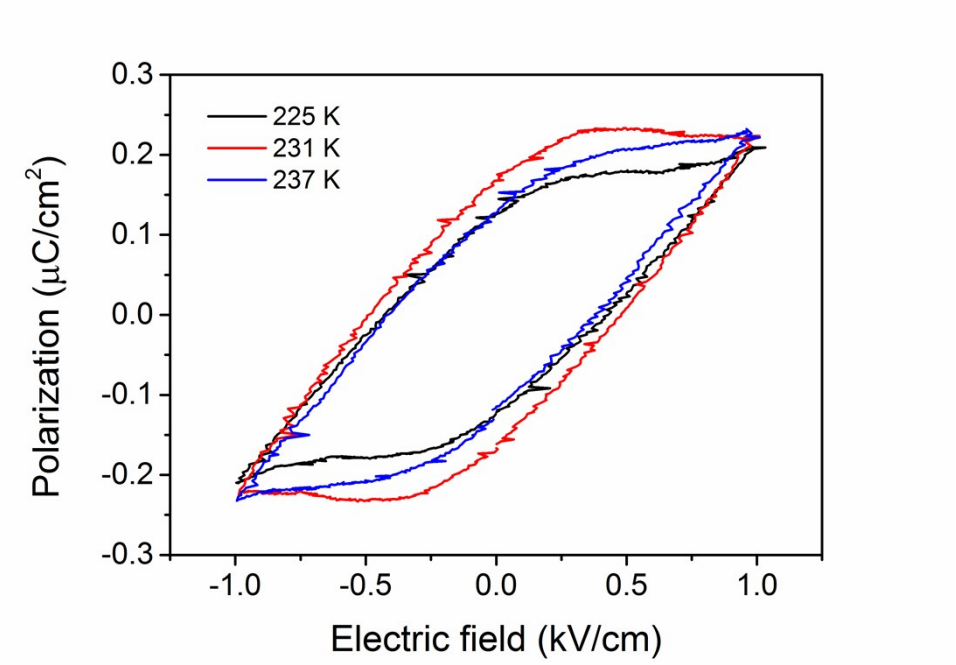

Fig. S4 PE loop measured at different temperature with 50 Hz frequency.

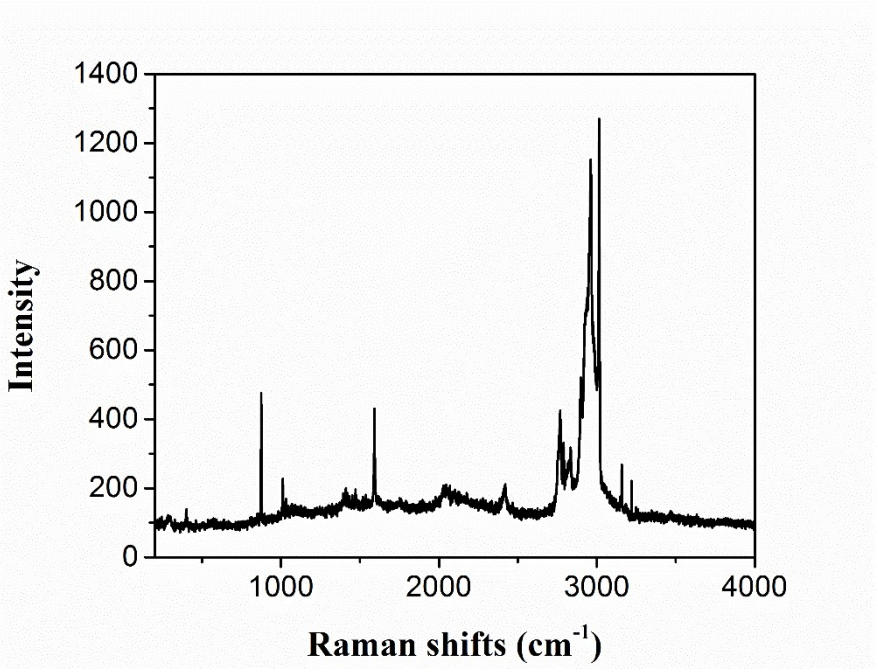

Fig. S5 Raman spectra of $DMAPbI_3$ measured at room temperature.

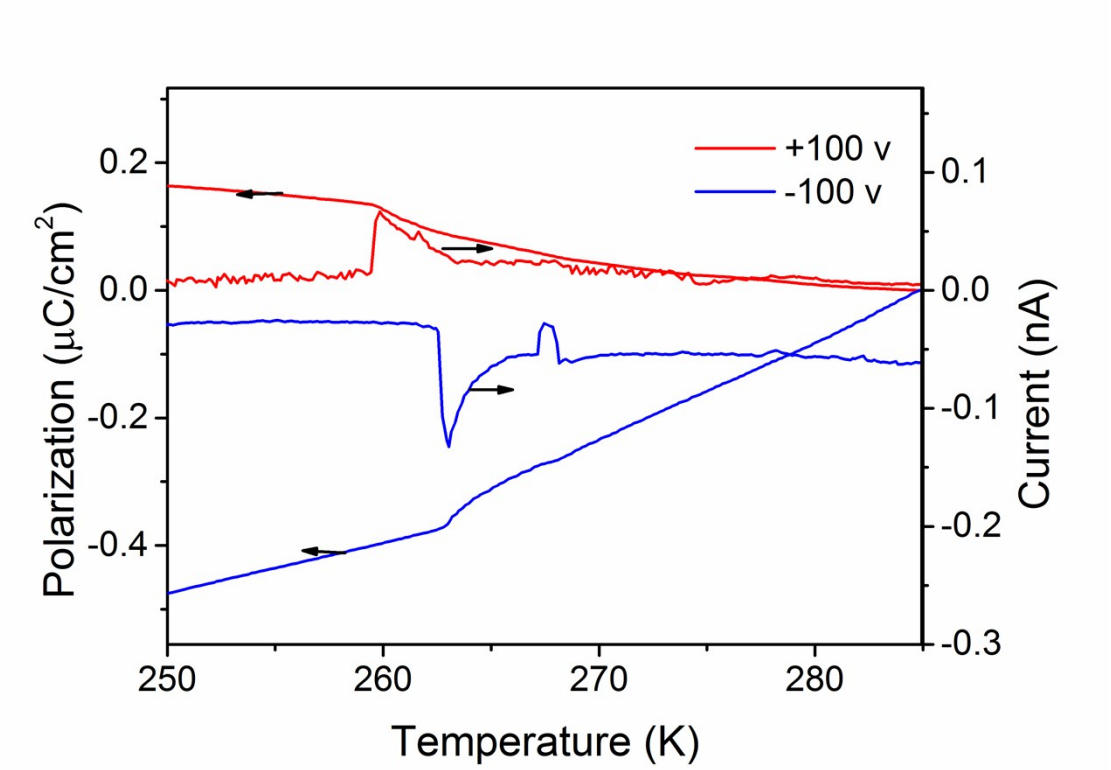

Fig. S6 Pyroelectric current and the corresponding spontaneous polarization of $DMAPbI_3$ measured after positive polarization and negative polarization with 10 K/min heating speed.

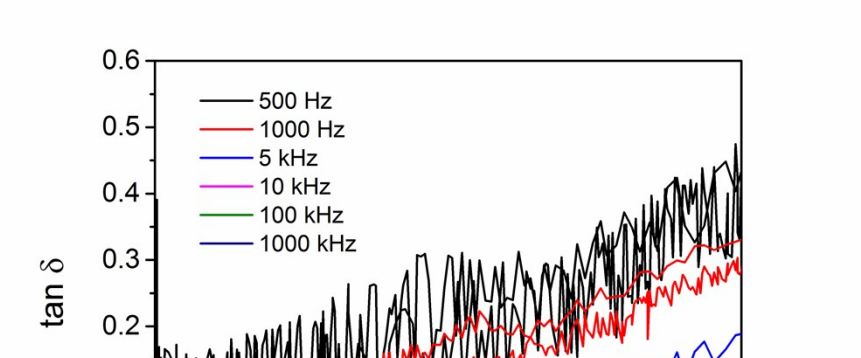

Fig. S7 The temperature dependent dielectric loss in the heating process and the cooling process.

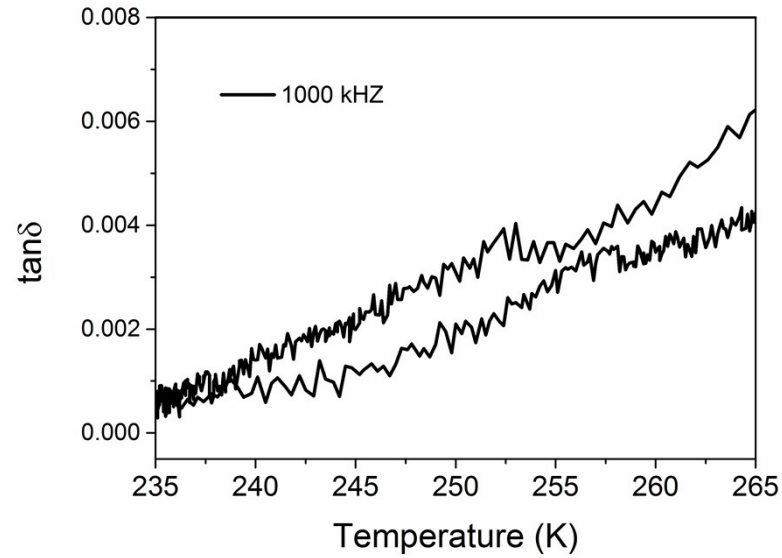

Fig. S8 The temperature dependent dielectric loss measured with 1000 kHz in the heating process and the cooling process